5-methyl-4-thia-1-heptyne

Other names: 2-Butyl propargyl sulfide
Inchi: InChI=1S/C7H12S/c1-4-6-8-7(3)5-2/h1,7H,5-6H2,2-3H3
InchiKey: GCNRFCHIMLFBMB-UHFFFAOYSA-N
Formula: C7H12S
SMILES: C#CCSC(C)CC
Mol. weight [g/mol]: 128.24

Physical Properties

Property code	Value	Unit	Source
gf	261.81	kJ/mol	Joback Method
hf	140.68	kJ/mol	Joback Method
hfus	17.47	kJ/mol	Joback Method
hvap	37.46	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.151		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	3392.03	kPa	Joback Method
rinpol	933.00		NIST Webbook
rinpol	933.00		NIST Webbook
tb	418.02	K	Joback Method
tc	624.16	K	Joback Method
tf	235.02	K	Joback Method
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.03	J/mol×K	418.02	Joback Method
cpg	229.56	J/mol×K	452.38	Joback Method
cpg	240.55	J/mol×K	486.73	Joback Method
cpg	251.01	J/mol×K	521.09	Joback Method
cpg	260.95	J/mol×K	555.45	Joback Method
cpg	270.39	J/mol×K	589.80	Joback Method
cpg	279.35	J/mol×K	624.16	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R144022&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume